

## Safety Data Sheet

according to Regulation (EC) No 1907/2006

## 4-Hydroxy-4-methyl-2-pentanone (Diacetone alcohol) for synthesis

Revision date: 02.08.2023

Product code: 25302

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1. Product identifier**

4-Hydroxy-4-methyl-2-pentanone (Diacetone alcohol) for synthesis

CAS No: 123-42-2  
Index No: 603-016-00-1  
EC No: 204-626-7

**1.2. Relevant identified uses of the substance or mixture and uses advised against****Use of the substance/mixture**

Laboratory chemical

Industrial uses: Uses of substances as such or in preparations at industrial sites

Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

**Uses advised against**

Do not use for private purposes (household).

**1.3. Details of the supplier of the safety data sheet**

Company name: AnalytiChem GmbH  
Street: Stempelstraße 6  
Place: D-47167 Duisburg  
Telephone: 0203/5194-0  
E-mail: info@analytichem.de  
Contact person: Abteilung Produktsicherheit  
E-mail: produktsicherheit@analytichem.de  
Internet: www.analytichem.de  
Responsible Department: Abteilung Produktsicherheit

Telefax: 0203/5194-290

Telephone: 0203/5194-107/117

**1.4. Emergency telephone number:**

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

**Further Information**

A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

**SECTION 2: Hazards identification****2.1. Classification of the substance or mixture****Regulation (EC) No 1272/2008**

Flam. Liq. 3; H226

Eye Irrit. 2; H319

Full text of hazard statements: see SECTION 16.

**2.2. Label elements****Regulation (EC) No 1272/2008**

Signal word: Danger

Pictograms:

**Hazard statements**

H225

Highly flammable liquid and vapour.

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H319 Causes serious eye irritation.

**Precautionary statements**

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233 Keep container tightly closed.

P280

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P337+P313 If eye irritation persists: Get medical advice/attention.

P403+P235 Store in a well-ventilated place. Keep cool.

**2.3. Other hazards**

No information available.

**SECTION 3: Composition/information on ingredients****3.1. Substances**Sum formula: (CH<sub>3</sub>)<sub>2</sub>C(OH)

Molecular weight: 116.16 g/mol

**Hazardous components**

CAS No	Chemical name	Quantity		
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
123-42-2	4-hydroxy-4-methylpentan-2-one			100 %
	204-626-7	603-016-00-1		
	Flam. Liq. 3, Eye Irrit. 2; H226 H319			

Full text of H and EUH statements: see section 16.

**Specific Conc. Limits, M-factors and ATE**

CAS No	EC No	Chemical name	Quantity	
	Specific Conc. Limits, M-factors and ATE			
123-42-2	204-626-7	4-hydroxy-4-methylpentan-2-one	100 %	
	oral: LD50 = 3002 mg/kg Eye Irrit. 2; H319: >= 10 - 100			

**Further Information**

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

**SECTION 4: First aid measures****4.1. Description of first aid measures****General information**

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

**After inhalation**

Provide fresh air.

If breathing is irregular or stopped, administer artificial respiration.

Call a physician immediately.

**After contact with skin**

Wash immediately with:

Water and soap

Take off immediately all contaminated clothing and wash it before reuse.

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#### After contact with eyes

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately.

#### After ingestion

Do NOT induce vomiting.  
Rinse mouth thoroughly with water.  
Call a physician immediately.

#### 4.2. Most important symptoms and effects, both acute and delayed

Depression of central nervous system  
Headache  
Dizziness  
Induces narcotic effect.  
Unconsciousness  
Impairment of vision

#### 4.3. Indication of any immediate medical attention and special treatment needed

No data available

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

#### Suitable extinguishing media

Water spray jet, Carbon dioxide (CO<sub>2</sub>), Foam, Extinguishing powder.

#### Unsuitable extinguishing media

no restriction

### 5.2. Special hazards arising from the substance or mixture

Combustible liquid.  
Vapours are heavier than air, spread along floors and form explosive mixtures with air.  
Hazardous combustion products  
In case of fire may be liberated:  
Carbon dioxide (CO<sub>2</sub>) Carbon monoxide

### 5.3. Advice for firefighters

Remove persons to safety. Do not inhale explosion and combustion gases.  
Avoid contact with skin, eyes and clothes.  
In case of fire: Wear self-contained breathing apparatus.  
Use water spray jet to protect personnel and to cool endangered containers.

#### Additional information

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.  
Suppress gases/vapours/mists with water spray jet.  
Move undamaged containers from immediate hazard area if it can be done safely.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

#### General advice

Keep away from sources of ignition - No smoking.  
This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators, and pagers which have not been certified as intrinsically safe).  
Take action to prevent static discharges.

#### For non-emergency personnel

Provide adequate ventilation.  
Use personal protection equipment.  
Avoid contact with skin, eyes and clothes.

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Remove persons to safety.  
Emergency procedures  
Do not breathe dust/fume/gas/mist/vapours/spray.

#### For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

#### 6.2. Environmental precautions

Do not allow to enter into surface water or drains.  
The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in high concentration.  
Danger of explosion

#### 6.3. Methods and material for containment and cleaning up

##### For containment

Cover drains.  
Prevent spread over a wide area (e.g. by containment or oil barriers).  
Collect in closed and suitable containers for disposal.  
Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

##### For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

##### Other information

Provide adequate ventilation.  
Do not breathe dust/fume/gas/mist/vapours/spray.  
Wear breathing apparatus if exposed to vapours/dusts/aerosols.

#### 6.4. Reference to other sections

Safe handling: see section 7  
Personal protection equipment: see section 8  
Disposal: see section 13

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

#### Advice on safe handling

Read label before use. Handle and open container with care.  
When using do not eat, drink, smoke, sniff. Keep container tightly closed.  
Use personal protection equipment. Use extractor hood (laboratory).  
Do not breathe gas/fumes/vapour/spray. Provide adequate ventilation.

#### Advice on protection against fire and explosion

Take action to prevent static discharges. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

#### Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.  
Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or drink.

#### Further information on handling

Take off immediately all contaminated clothing and wash it before reuse.  
If handled uncovered, arrangements with local exhaust ventilation have to be used.  
Draw up and observe skin protection programme.  
Wash hands and face before breaks and after work and take a shower if necessary.

### 7.2. Conditions for safe storage, including any incompatibilities

#### Requirements for storage rooms and vessels

Keep container tightly closed. Keep in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

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#### Hints on joint storage

Do not store together with:  
Oxidising agent

#### Further information on storage conditions

Vapours may form explosive mixtures with air.  
storage temperature < +30°C.

#### 7.3. Specific end use(s)

Laboratory use Laboratory chemical

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

#### Occupational exposure limits

CAS No	Substance	ppm	mg/m <sup>3</sup>	fib/cm <sup>3</sup>	Category	Origin
123-42-2	4-Hydroxy-4-methyl-2-pentanone	50	240		TWA (8 h)	

#### DNEL/DMEL values

CAS No	Substance	Exposure route	Effect	Value
123-42-2	4-hydroxy-4-methylpentan-2-one			
Worker DNEL, long-term		inhalation	systemic	59,2 mg/m <sup>3</sup>
Worker DNEL, acute		inhalation	local	240 mg/m <sup>3</sup>
Worker DNEL, long-term		dermal	systemic	840 mg/kg bw/day
Consumer DNEL, long-term		inhalation	systemic	10,4 mg/m <sup>3</sup>
Consumer DNEL, long-term		dermal	systemic	60 mg/kg bw/day
Consumer DNEL, long-term		oral	systemic	3 mg/kg bw/day

#### PNEC values

CAS No	Substance	Value
123-42-2	4-hydroxy-4-methylpentan-2-one	
Freshwater		2 mg/l
Freshwater (intermittent releases)		1 mg/l
Marine water		0,2 mg/l
Freshwater sediment		9,06 mg/kg
Marine sediment		0,91 mg/kg
Micro-organisms in sewage treatment plants (STP)		10 mg/l
Soil		0,63 mg/kg

### 8.2. Exposure controls

#### Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment.

If handled uncovered, arrangements with local exhaust ventilation have to be used.

#### Individual protection measures, such as personal protective equipment

##### Eye/face protection

Suitable eye protection: goggles.

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#### Hand protection

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: [vertrieb@kcl.de](mailto:vertrieb@kcl.de) With specification (test according to EN374):

By long-term hand contact

Trade name/designation KCL 897 Butoject®

Suitable material: Butyl caoutchouc (butyl rubber) 0,3 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Trade name/designation KCL 730 Camatril® Velours

Suitable material: NBR (Nitrile rubber) 0,4 mm

Wearing time with occasional contact (splashes): > 120 min

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types. This recommendation applies only to the product stated in the safety data sheet (>, <) supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

#### Skin protection

Flame-retardant protective clothing. Wear anti-static footwear and clothing

#### Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

Filtering device with filter or ventilator filtering device of type: ABEK

#### Environmental exposure controls

Do not empty into drains.

The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in higher concentration.

Danger of explosion

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Physical state:	Liquid
Colour:	light yellow
Odour:	characteristic
Odour threshold:	No data available
Melting point/freezing point:	No data available
Boiling point or initial boiling point and boiling range:	166 °C
Flammability:	not applicable
Lower explosion limits:	1,8 vol. %
Upper explosion limits:	6,9 vol. %
Flash point:	58 °C
Auto-ignition temperature:	643 °C
Decomposition temperature:	not determined
pH-Value:	No data available
Viscosity / kinematic:	No data available
Water solubility:	No data available
Solubility in other solvents	
not determined	
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	No data available

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Dispersion stability:	No data available
Vapour pressure: (at 20 °C)	1,29 hPa
Vapour pressure:	No data available
Density (at 25 °C):	0,931 g/cm <sup>3</sup>
Relative density:	No data available
Bulk density:	No data available
Relative vapour density:	not determined
Particle characteristics:	No data available

#### 9.2. Other information

##### Information with regard to physical hazard classes

###### Explosive properties

Vapours can form explosive mixtures with air.

###### Sustaining combustion:

No data available

###### Self-ignition temperature

Solid:

not applicable

Gas:

not applicable

###### Oxidizing properties

Not oxidising.

##### Other safety characteristics

###### Evaporation rate:

not determined

###### Solvent separation test:

No data available

###### Solvent content:

No data available

###### Solid content:

not determined

###### Sublimation point:

No data available

###### Softening point:

No data available

###### Pour point:

No data available

###### No data available:

###### Viscosity / dynamic:

No data available

###### Flow time:

No data available

##### Further Information

No data available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

Vapours can form explosive mixtures with air.

### 10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

### 10.3. Possibility of hazardous reactions

Oxidising agent

Alkali (lye)

### 10.4. Conditions to avoid

Keep away from sources of heat (e.g. hot surfaces), sparks and open flames.

Vapours can form explosive mixtures with air.

### 10.5. Incompatible materials

No data available

### 10.6. Hazardous decomposition products

Hazardous combustion products

In case of fire may be liberated: Carbon dioxide (CO<sub>2</sub>) Carbon monoxide

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**Further information**

No data available

**SECTION 11: Toxicological information**

**11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008**

**Toxicokinetics, metabolism and distribution**

No data available

**Acute toxicity**

Based on available data, the classification criteria are not met.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
123-42-2	4-hydroxy-4-methylpentan-2-one				
	oral	LD50 3002 mg/kg	Rat	Study report (1978)	OECD Guideline 401

**Irritation and corrosivity**

Causes serious eye irritation.

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

**Sensitising effects**

Based on available data, the classification criteria are not met.

**Carcinogenic/mutagenic/toxic effects for reproduction**

Based on available data, the classification criteria are not met.

**STOT-single exposure**

Based on available data, the classification criteria are not met.

**STOT-repeated exposure**

Based on available data, the classification criteria are not met.

**Aspiration hazard**

Based on available data, the classification criteria are not met.

**Information on likely routes of exposure**

No data available

**Specific effects in experiment on an animal**

No data available

**Additional information on tests**

No data available

**Practical experience**

No data available

**11.2. Information on other hazards**

**Endocrine disrupting properties**

No data available

**Other information**

Depression of central nervous system

Headache

Dizziness

Induces narcotic effect.

Unconsciousness

Impairment of vision

**Further information**

Prolonged or repeated skin contact may cause removal of natural fat from the skin resulting in dermatitis (skin inflammation).



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**SECTION 12: Ecological information**

**12.1. Toxicity**

Based on available data, the classification criteria are not met.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h]   [d]	Species	Source	Method
123-42-2	4-hydroxy-4-methylpentan-2-one					
	Acute fish toxicity	LC50 > 100 mg/l	96 h	Oryzias latipes	Study report (1997)	OECD Guideline 203
	Acute algae toxicity	ErC50 > 1000 mg/l	72 h	Pseudokirchneriella subcapitata	Study report (1997)	OECD Guideline 201
	Acute crustacea toxicity	EC50 > 1000 mg/l	48 h	Daphnia magna	Study report (1997)	OECD Guideline 202
	Crustacea toxicity	NOEC 100 mg/l	14 d	Daphnia magna	Study report (1997)	OECD Guideline 211
	Acute bacteria toxicity	(EC50 > 1000 mg/l)	3 h	activated sludge, domestic	Study report (2012)	OECD Guideline 209

**12.2. Persistence and degradability**

No data available

**12.3. Bioaccumulative potential**

No data available

**Partition coefficient n-octanol/water**

CAS No	Chemical name	Log Pow
123-42-2	4-hydroxy-4-methylpentan-2-one	1,9

**12.4. Mobility in soil**

No data available

**12.5. Results of PBT and vPvB assessment**

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

**12.6. Endocrine disrupting properties**

This substance does not have endocrine disrupting properties with respect to non-target organisms.

**12.7. Other adverse effects**

No data available

**Further information**

Avoid release to the environment.  
Do not allow to enter into surface water or drains.

**SECTION 13: Disposal considerations**

**13.1. Waste treatment methods**

**Disposal recommendations**

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.  
Send to a physico-chemical treatment facility under observation of official regulations. Do not empty into drains.

**Contaminated packaging**

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.  
Handle contaminated packages in the same way as the substance itself.

**SECTION 14: Transport information**

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**Land transport (ADR/RID)**

<b>14.1. UN number or ID number:</b>	UN 1148
<b>14.2. UN proper shipping name:</b>	DIACETONE ALCOHOL
<b>14.3. Transport hazard class(es):</b>	3
<b>14.4. Packing group:</b>	III
Hazard label:	3
Classification code:	F1
Limited quantity:	5 L
Excepted quantity:	E1
Transport category:	3
Hazard No:	30
Tunnel restriction code:	D/E

**Inland waterways transport (ADN)**

<b>14.1. UN number or ID number:</b>	UN 1148
<b>14.2. UN proper shipping name:</b>	DIACETONE ALCOHOL
<b>14.3. Transport hazard class(es):</b>	3
<b>14.4. Packing group:</b>	III
Hazard label:	3
Classification code:	F1
Limited quantity:	5 L
Excepted quantity:	E1

**Marine transport (IMDG)**

<b>14.1. UN number or ID number:</b>	UN 1148
<b>14.2. UN proper shipping name:</b>	DIACETONE ALCOHOL
<b>14.3. Transport hazard class(es):</b>	3
<b>14.4. Packing group:</b>	III
Hazard label:	3
Special Provisions:	223
Limited quantity:	5 L
Excepted quantity:	E1
EmS:	F-E, S-D

**Air transport (ICAO-TI/IATA-DGR)**

<b>14.1. UN number or ID number:</b>	UN 1148
<b>14.2. UN proper shipping name:</b>	DIACETONE ALCOHOL
<b>14.3. Transport hazard class(es):</b>	3
<b>14.4. Packing group:</b>	III
Hazard label:	3
Special Provisions:	A3
Limited quantity Passenger:	10 L
Passenger LQ:	Y344
Excepted quantity:	E1
IATA-packing instructions - Passenger:	355
IATA-max. quantity - Passenger:	60 L
IATA-packing instructions - Cargo:	366
IATA-max. quantity - Cargo:	220 L

**14.5. Environmental hazards**

ENVIRONMENTALLY HAZARDOUS: No

**14.6. Special precautions for user**

Warning: Combustible liquid.

**14.7. Maritime transport in bulk according to IMO instruments**

not applicable

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#### SECTION 15: Regulatory information

##### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

###### EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 40

Information according to 2012/18/EU  
(SEVESO III):

P5c FLAMMABLE LIQUIDS

###### National regulatory information

Employment restrictions:

Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC).

Water hazard class (D):

1 - slightly hazardous to water

##### 15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

#### SECTION 16: Other information

##### Changes

This data sheet contains changes from the previous version in section(s): 9,12.

##### Abbreviations and acronyms

ADR: Accord européen sur le transport des marchandises dangereuses par Route  
(European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service

LC50: Lethal concentration, 50%

LD50: Lethal dose, 50%

Flam. Liq: Flammable liquid

Eye Irrit: Eye irritation

##### Relevant H and EUH statements (number and full text)

H225 Highly flammable liquid and vapour.

H226 Flammable liquid and vapour.

H319 Causes serious eye irritation.

##### Further Information

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material. The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

The receiver of our product is singularly responsible for adhering to existing laws and regulations.